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COMPARISON OF A FEW STATISTICAL METHODS FOR VALIDATION

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Introduction

Many institutions are using a sophisticated statistical methodology to validate criticality safety computer codes in compliance with the ANSI/ANS-8.1 and -8.24 standards (Ref. 1 and 2). Here a few similar statistical methods are compared, namely, the USLSTATS method developed by the Oak Ridge National Laboratory (ORNL), the Washington Safety Management Solutions (WSMS) method, and the GE USLSA method. These methods use the 'trending analysis' technique, namely, the derivation of bias for an application is correlated to biases for benchmark experiments. The methods use regression techniques to identify trends. But they differ in choice and calculation of specific "regression parameters".

Each method either provides directly or supports derivation of an Upper Subcritical Limit (USL), also often designated as "k_{safe}". USL can be defined as

$$USL = 1 + \beta - \Delta\beta - MSM$$

Where

β = the calculational bias = k_c -1,

k_c = the mean value of k_{eff} resulting from the calculation of critical benchmark experiments using a specific calculational method and set of cross section data.

$\Delta\beta$ = is the bias uncertainty which may include uncertainties in the critical experiments, statistical and or convergence uncertainties in the benchmark calculations, uncertainties due to extrapolation beyond the range of experimental data, and uncertainties due to limitations or weaknesses in the geometrical or nuclear modeling of the critical experiments.

MSM = Minimum Subcritical Margin which is the administrative and /or statistical margins applied to an application such that, if the calculated k for a system satisfies the following inequality, the system is subcritical with a high degree of confidence.

$$k = k_{eff} + 2\sigma < USL$$

ORNL USLSTATS Method

The ORNL USLSTATS program uses two methods — (1) confidence band with administrative margin and (2) single-sided uniform-width closed interval — to calculate the USL based on a set of user-supplied k_{eff} values and corresponding values of an associated system parameter (independent variable). The USLSTATS programs is described and discussed in References 3, 4, 5, and 6.

Method 1: Confidence Band with Administrative Margin

This method applies a statistical calculation of the bias and its uncertainty as a linear fit of critical experiment benchmark data plus an administrative margin. A linear regression fit is applied to a set of calculated k_{eff} and uncertainty values, k,(x), for a set of critical experiments. The lower confidence band is then calculated. The width of this band is determined statistically based on the existing data and a specified level of confidence. The greater the standard deviation in the data or the larger the confidence desired, the larger the band width will be. This confidence band, W, accounts for uncertainties in the experiments, the calculational approach, and calculational data (e.g., cross sections), and is therefore a statistical basis for $\Delta\beta$, the uncertainty in the value of β. The confidence band calculation is discussed in detail in Reference 3.

The USL is based on an additional margin of subcriticality (MSM), which provides assurance of subcriticality. In Method 1, the MSM is given an arbitrary administrative value; a minimum of 0.05 is recommended for application to transportation and storage packages and usually a minimum value of 0.02 is recommended for other applications.

Method 2: Lower Tolerance Band (LTB) Approach

The Lower Tolerance Band (LTB) approach is sometimes called Single-Sided Uniform Width Closed Interval Approach. This is a statistical technique with a rigorous basis and is applied in order to determine a combined lower confidence band plus subcritical margin. In other words, in the administrative margin approach, MSM and $\Delta\beta$ are determined independently, while in the LTB method, a combined statistical lower bound is determined.

The details of this methodology are given in Reference 3. The purpose of this method is to determine a uniform tolerance band over a specified closed interval for a linear least-squares model. The level of confidence, α, in the limit being calculated is typically in the range from 0.90 to 0.999.

The USL Method 2 is based on the equation

$$USL_2\,(x) = 1.0 - (C_{\alpha/P} .\ s_p) + \beta(x),$$

where s_p is the pooled variance of k_c. The term $C_{\alpha/P} .\ s_p$ provides a band for which there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band.

For example, a $C_{95/99.5}$ multiplier produces a USL for which there is a 95% confidence that 995 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the USL. The analysis is over the closed interval from x = a to x = b.

$C_{\alpha/P}$ depends on z_P and χ^2, where z_P is the Student t statistic depending on n and P and χ^2 is the chi square distribution, a function of n-2 and α.

This approach provides a statistically based subcritical margin, Δk_m which can be determined as the difference $(C_{\alpha/P} .\ s_p)$ - W. In criticality safety applications, such a statistically determined approach generally, but not necessarily, yields a margin of less than 0.05, which serves to illustrate the adequacy of the administrative margin. The recommended purpose of Method 2 is to apply it in tandem with Method 1 to verify that the administrative margin is conservative relative to a purely statistical basis. This concurrent application of Method 2 is especially important when a limited number of data points are used in determination of k,(x), or when the calculated values have a large standard deviation.

WSMS Method

The WSMS method (described in References 7 and 8) uses an EXCEL spreadsheet (bias.xls) incorporating a statistical weighted least-squares regression analysis to derive a Single-sided Lower Tolerance Band (LTB) and a Single-sided Lower Confidence Band (LCB). Regression analyses involve the fitting of a line or curve to the calculated k_{eff} values against some independent variable. Linear and polynomial fits to the k_{eff} data as a function of the independent variable are used. The fitted equation is of the form: $y = a + bx$. The linear fit techniques are based on methods presented in Natrella (Ref. 9) and in Bevington (Ref. 10). A non-linear equation is handled by "transforming" the non-linear equation into a linear equation and then solving for the applicable equation parameters. Trending of the data is based on the fits. The linear correlation coefficient (r) is a quantitative measure of the degree that a linear relationship exists between two sets of variables. The correlation coefficient is often expressed as a squared term, r^2. The closer r^2 approaches the value of 1, the better the fit of the data to the linear equation.

User selection of the biased k_{eff} value, k_{be}, representation depends on the understanding of the relationship between the independent variable and the calculated k_{eff} values for selected sets of benchmark experiments. If the reason for the trend in bias is known, the LCB defines the region where the true bias is expected to be, within a prescribed degree of confidence. The LCB has the smallest bias and bias uncertainty. If the reason for the trend in bias is not known, the more conservative LTB defines the region above which a proportion of bias will lie for some prescribed degree of confidence. A confidence factor of 95% and a proportion factor of 95% are normally used.

A Single-sided Lower Tolerance Limit (LTL) is derived if the derived fit is not well correlated with the k_{eff} values (i.e., no clear trend) and the distribution of k_{eff} values is normal based on a normalcy test. This statistical treatment is valid only over the area of applicability of the benchmark experiments. If a fit is not correlated, the k_{eff} value distribution is not normal, or less than 10 experiment configurations are in the analyzed set of data, k_{be} is determined by a non-parametric technique. The Shapiro-Wilk test and the Chi-square test are used to determine if the k_{eff} data are normally distributed.

The statistical weighting, $W=1/\sigma_i^2$, is based on the combination of the experimental uncertainty (σ_e) and calculational statistical uncertainty (σ_s) as a total uncertainty, σ_i.

$$\sigma_i = \sqrt{\sigma_{e,i}^2 + \sigma_{s,i}^2}$$

where the subscript (*i*) refers to an individual benchmark calculation.

Benchmark experiments used for validation may not be exactly critical. Normalized k_{eff} valves are used in the k_{be} determination. The calculated k_{eff} values are normalized to the experimental values as follows:

$$k_{eff}(\text{normalized}) = k_{eff}(\text{calculated}) / k_{eff}(\text{experimental}).$$

Often, available experimental data do not completely cover the range of applicability of the problem to be analyzed. One of the advantages of performing a fit to benchmark validation calculations is the ability to extrapolate beyond the area of applicability. Extrapolation cannot be performed if using an LTL, without applying additional margin. However, if a good fit of the data to an independent variable is possible, then a LCB or LTB can be used for extrapolation. Extrapolation is usually limited to +/- 5% of most independent variables. The WSMS method also uses a Non-Parametric Technique for data that do not follow a normal distribution.

The derived biased k_{eff} functions or values determined with the WSMS method do not include an MSM. The MSM is determined by the NCS analyst for his specific system during determination of k_{safe} to be used in the inequality comparison, $k = k_{eff} + 2\sigma < k_{safe}$.

Figure 1 demonstrates the general relationships for the various derived functions.

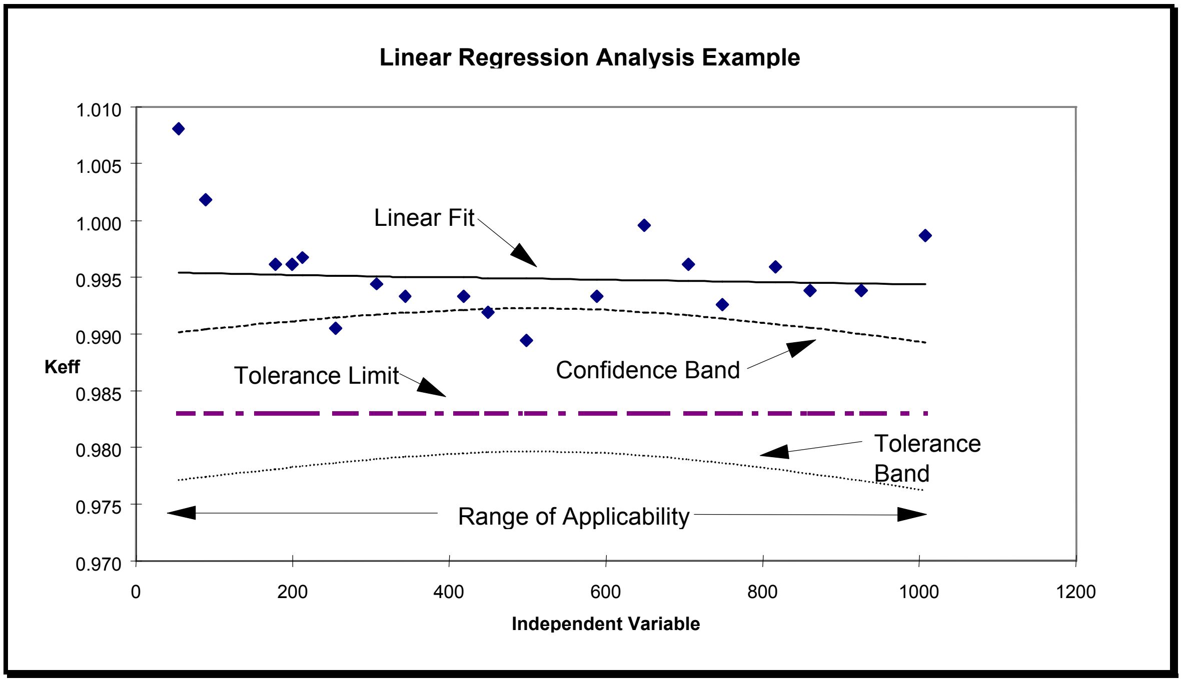

Figure 1 - Examples of WSMS Methodology

GEH USLSA Method

The GEH methodology (USLSA) consists of the weighted linear/nonlinear least-squares regression for the bias and three statistical interval methods (Single-Sided Lower Confidence Band, Single-Sided Lower Tolerance Band, and Single-Sided Lower Tolerance Limit) for the bias uncertainty. The bias uncertainty can be determined either analytically for linear regression or stochastically for nonlinear regression. USLSA provides rigorous statistical tests on the validity of validation model, including residual assumptions of regression model, magnitude of model effect, goodness-of-fit, model significance and intended model extrapolations. The methodology is described in References 11 and 12.

Four statistical approaches are in the GEH method. They are: (1) single-sided lower confidence band (SSLCB), (2) single-sided lower tolerance band (SSLTB), (3) single-sided lower tolerance limit (SSLTL), and (4) non-parametric limit (NPL).

Method 1: Single-Sided Lower Confidence Band (SSLCB) Approach

When a relationship between a calculated k_{eff} and an independent parameter of a system or process can be determined, a single-sided lower confidence band may be used. The USL derived with this method as a function of some trending parameter x is defined as

$$USL(x) = \bar{k}_e + b(x) - W_c - \Delta k_m$$

where, $\bar{k}_e$ is the weighted mean of measured k_{eff}; $b(x)$ is a fit function of the calculational bias; Δk_m *is* the *minimum margin of subcriticality* (MMS); and W_c is the maximum confidence bandwidth over the range of the trending parameter and provides a statistical estimate for the uncertainty in the bias. W_c is defined as

$$W_c = \max\left[t_{1-\alpha,v}\, s_p \sqrt{1 + L(x)' S^{-1} L(x)}\right]$$

where, $t_{1\text{-}\alpha,v}$ is a 100(1- α)% of the inverse of central t cumulative distribution with v degrees of freedom; $L(x)$ is the coefficient partial derivative vector of $b(x)$; S is the design matrix; s_p^2 is the pooled variance.

The SSLCB approach is better suited to a set of benchmarks when a clear trend with a high goodness-of-fit is present and the trend is explained by the physics of the data. It is appropriate for determining the USL used routinely for a small number of future k_{eff} calculation for a system or process design.

Method 2: Single-Sided Lower Tolerance Band (SSLTB) Approach

The USL established by the SSLTB approach is similar to the SSLCB approach, except that W_c is replaced with W_t, the maximum tolerance bandwidth over the range of the trending parameter. The tolerance band can provide more conservative estimates of bias uncertainties than the confidence band. A Monte Carlo estimation for the single-sided lower tolerance band is developed to overcome the difficulty in calculating tolerance factors for nonlinear regression fitting of $b(x)$.

The SSLTB approach is better suitable for typical routine criticality safety calculation in which USLs are estimated once and applied to a large and potentially unknown number of future observation decisions, as well as for use in extrapolation of results.

Method 3: Single-Sided Lower Tolerance Limit (SSLTL) Approach

The SSLTL approach is used when there are no trends apparent in the calculated critical benchmark results. It requires the calculated k_{eff} data to have a normal distribution. The USL established by the SSLTL approach is similar to the SSLTB approach, except that bias is a weighted mean ($\bar{b}$) instead a function ($b(x)$), i.e.,

$$USL = \bar{k}_e + \bar{b} - W_t - \Delta k_m$$

The tolerance bandwidth, W_t, is given by

$$W_t = C_{(1-\alpha)/P} \cdot s_p$$

where, $C_{(1\text{-}\alpha)/P}$ is the single-sided tolerance factor for the normal distribution.

Method 4: Non-Parametric Limit (NPL) Approach

In cases where the calculated k_{eff} data (non-trending data) or the residuals of bias regression (trending data) fail the normality test, the NPL approach should be applied. This statistical technique is based on a rank order analysis of the data. The USL determined by this approach is given by

$$USL = k_{min} - \Delta k_{min} - \Delta k_{np}$$

where, k_{min} is the smallest k_{eff} value in the data set; Δk_{min} is the overall uncertainty for k_{min}; Δk_{np} is the non-parametric margin which is a function of the degree of confidence for a given sample size.

The GEH method tests the validity of the linear or nonlinear regression model of the bias. Multiple statistical tests are rigorously performed on residual assumptions (normality, independence and zero mean of population error), magnitude of model effect (R^2 and adjusted R^2), goodness-of-fit (χ^2 test and reduced χ^2) and model significance (F test). In addition, a leverage statistic is included in the SSLCB and SSLTB approaches to provide a maximal allowable range for the extrapolation of trending variable.

Methodology Comparisons

The three validation methodologies were applied to two sets of benchmark experiment calculations to provide comparisons of the techniques. One benchmark experiment set involved plutonium metal experiments, comprised of single units and arrays of units, with the k_{eff} values calculated by the MCNP 5 code. The other benchmark experiment set involved Low Enriched Uranium (LEU) experiments, with the k_{eff} values calculated by the GE GEMER code.

Calculated k_{eff} and Independent Data Values for Benchmark Experiments

Table 1 summarizes the calculated k_{eff} values, the calculated statistical uncertainty, the experimental k_{eff} values and uncertainties, and the independent variable for 67 plutonium metal experiments selected from the International Benchmark Handbook of Evaluated Criticality Safety Benchmark Experiments (Ref. 13). These experiments were comprised of single units and arrays of units, with the k_{eff} values calculated by the MCNP 5 code, using the ENDF/B-VI (.66c) cross section library (where available), running on SURYA, which is a LLNL HP UNIX Workstation. The MCNP 5 output tabulated the energy corresponding to the average neutron lethargy causing fission (called EALF herein) which was used as the independent variable for the analysis. PMF in the experiment descriptor stands for PU-METAL-FAST from the benchmark evaluation identification number.

Table 2 correspondingly summarizes the calculated k_{eff} values, the calculated statistical uncertainty, the experimental k_{eff} values and uncertainties, and the independent variable for 75 LEU and IEU experiments with the k_{eff} and statistical uncertainty values calculated by the GE GEMER code. The experiments are from evaluations in the ICSBEP Handbook and References 14, 15, and 16. The independent variable is the moderator to fissile ratio, H/X (i.e., H/U-235 atomic ratio).

Tables 3, 4, and 5 present summaries of the results of applying these three validation methods to the two sets of benchmark experiments. Values for various parameters (normality, correlation coefficient, statistical components, etc. provided by the methods are shown along with the equations of the regression fits and the equations representing the biased k_{eff} functions. The ranges of the biased k_{eff} functions (in some cases extrapolated) are also shown. The USL-1 function from the USLSTATS method includes an administrative margin of 0.02.

Figures 2 and 3 show the k_{eff} distributions as a function of the independent variables (EALF and H/X, respectively) along with the regression fit functions from the three methods, USLSTATS USL-1, WSMS LTB (W-LTB), and the GEH USLSA functions SSLCB and SSLTB. In Figures 2 and 3, the administrative margin in the USLSTATS USL-1 function has been removed (i.e., USL-1 increased by 0.02) to allow direct comparison of the regression functions. All methods provide biased k_{eff} functions whose values are less than almost all the experimental k_{eff} values. The results from each methodology are briefly discussed in the following.

USLSTATS Methodology

Plutonium Metal Experiments

USLSTATS indicates the k_{eff} data are normally distributed (Chi value of 4.5672 < upper bound of 9.49 indicates normal). Only a linear regression fit is provided by USLSTATS. For EALF ≤ 0.15196, the USL-1 function is a constant, 0.9718. Comparisons of the USL-1 and USL-2 functions and the ranges of their values demonstrate that an MSM of 0.02 is reasonable. The minimum USL-1 value is 0.9690. The USL (or k_{safe}) to be used in a nuclear criticality safety analysis can be taken either as the minimum USL-1 value, 0.9690, or as the USL-1 function shown in Table 3.

Low-Enriched Uranium Experiments

USLSTATS indicates the k_{eff} data are normally distributed (Chi value of 5.7333 < upper bound of 9.49 indicates normal). Only a linear regression fit is provided by USLSTATS. Comparisons of the USL-1 and USL-2 functions and the ranges of their values demonstrate that an MSM of 0.02 is reasonable. The minimum USL-1 value is 0.9552. The USL (or k_{safe}) to be used in a nuclear criticality safety analysis can be taken either as the minimum USL-1 value, 0.9552, or as the USL-1 function shown in Table 3.

WSMS Methodology

Plutonium Metal Experiments

The WSMS method indicates the k_{eff} data are normally distributed (Shapira-Wilk test value greater than test criterion, 0.9799 > 0.9643). Both linear and polynomial regression functions were tested. The polynomial regression fit is not significantly better than the linear regression fit. The linear function is visually a reasonable fit to the calculated k_{eff} values, but the correlation coefficient (R^2 = 0.0415) indicates a very low degree of correlation between the fit and the calculated k_{eff} values, likely due to the large variation in the k_{eff} values (see Figure 2). Since the calculated k_{eff} values are normally distributed and the linear regression fit is not well correlated, the LTL value of 0.9890 would be applied as the biased k_{eff} value. The LTL compares well with the LTB and LCB ranges of 0.9866 to 0.9883 and 0.9964 to 0.9981, respectively. The WSMS method does not directly determine the bias and bias uncertainty. Applying an MSM of 0.02 to the LTL value of 0.9890 yields 0.9690, in good agreement with the minimum USL-1 value. Extrapolation is not allowed without additional AoA margin.

Low-Enriched Uranium Experiments

The WSMS method indicates the k_{eff} data are normally distributed (S-W test value greater than test criterion, 0.9704 > 0.9675). Both linear and polynomial regression functions were tested. The polynomial regression fit is not significantly better than the linear regression fit. The linear function is visually a reasonable fit to the calculated k_{eff} values, but the correlation coefficient (R^2 = 0.1342) indicates a low degree of correlation between the fit and the calculated k_{eff} values, likely due to the large variation in the k_{eff} values (see Figure 3). Since the calculated k_{eff} values are normally distributed and the linear regression fit is not well correlated, the LTL value of 0.9858 would be applied as the biased k_{eff} value. The LTL compares well with the LTB and LCB ranges of 0.9824 to 0.9862 and 0.9909 to 0.9948, respectively. The WSMS method does not directly determine the bias and bias uncertainty. Applying an MSM of 0.02 to the LTL value of 0.9858 yields 0.9658, somewhat greater than, but reasonably consistent with, the minimum USL-1 value. Extrapolation is not allowed without additional AoA margin.

GEH USLSA Methodology

Plutonium Metal Experiments

A linear regression model is used to fit to the calculated k_{eff} values. Higher order polynomial or exponential function fittings do not improve the quality of regression. The R^2 and $R_{adj}{}^2$ values (0.006 and –0.0306) indicate that the magnitude of correlation between the model-predicted and calculated k_{eff} values is small. Both *F*-test and $\chi 2$ tests also show that the regression model is not statistically significant, although it is statistically valid per the residual normality test. The normality of residual assures the validity of the USL and the bias uncertainty determined by the SSLCB and SSLTB methods. In the extrapolated range of EALF (0, 1.3476), the minimal USL is 0.9911 for SSLCB and 0.9795 for SSLTB with corresponding bias uncertainties of 0.008 and 0.0197, respectively.

Since the calculated k_{eff} values are normally distributed and the linear regression model is statistically insignificant, the SSLTL method can be applied. The SSLTL of 0.9817 with a bias uncertainty of 0.0175 is appropriate for these experiments. Applying an MSM of 0.02 to the SSLTL of 9817 yields 0.9617, in good agreement with the minimum USL-1 value. Extrapolation is not allowed without additional AoA margin.

Low-Enriched Uranium Experiments

A linear regression model is used to fit to the calculated k_{eff} values. Higher order polynomial or exponential function fittings do not help improve the quality of regression. The R^2 and $R_{adj}{}^2$ values (0.1411 and 0.1172) show that about 12% variation in k_{eff} can be explained by the regression model. *F*-test, $\chi 2$ and residual normality tests also indicate the statistical validity and significance of the model. In the extrapolated range of $H/^{235}U$ (0, 1485), the minimal USL is 0.9840 for SSLCB and 0.9700 for SSLTB with corresponding bias uncertainties of 0.0096 and 0.0236, respectively.

Since the calculated k_{eff} values are normally distributed, the SSLTL method can be applied. A USL of 0.9732 with a bias uncertainty of 0.0213 is appropriate for these experiments. Applying an MSM of 0.02 to the SSLTL of 9732 yields 0.9532, in reasonable agreement with the minimum USL-1 value. Extrapolation is not allowed without additional AoA margin.

Conclusion

All three methods provide a statistically-based linear regression analysis to validate a computer code. Although the specific details of the statistical analysis vary between the three methods, the methods yield similar results for the biased k_{eff} function or value.

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Table 1: Benchmark Set 1, Pu Metal– MCNP5 Calculations

Experiment Descriptor	No.	File ID	Expt. k_{eff}	Expt. σ	MCNP k_{eff}	MCNP σ	EALF (MeV)
PMF-001	1	pmf001	1.0000	0.0020	0.99756	0.00056	1.2564E+00
PMF-002	2	pmf002	1.0000	0.0020	0.99896	0.00061	1.2720E+00
PMF-003	3	pmf003c1r	1.0000	0.0030	0.99960	0.00061	1.2501E+00
	4	pmf003c2r	1.0000	0.0030	0.99403	0.00067	7.3208E-01
	5	pmf003c3r	1.0000	0.0030	0.99348	0.00052	1.2516E+00
	6	pmf003c4r	1.0000	0.0030	0.99514	0.00072	6.5915E-01
	7	pmf003c5r	1.0000	0.0030	0.99513	0.00061	1.2537E+00
PMF-004	8	p-mt008	1.0000	0.0030	0.99394	0.0007	1.2091E+00
	9	p-mt009	1.0000	0.0030	0.99495	0.0007	1.1685E+00
	10	p-mt010	1.0000	0.0030	0.99441	0.00065	1.1674E+00
	11	p-mt011	1.0000	0.0030	0.99388	0.00065	1.1627E+00
	12	p-mt012	1.0000	0.0030	0.99449	0.00071	1.1665E+00
	13	p-mt013	1.0000	0.0030	0.99449	0.00068	1.1699E+00
	14	p-mt014	1.0000	0.0030	0.99344	0.00065	1.2341E+00
	15	p-mt015	1.0000	0.0030	0.99539	0.00067	1.2230E+00
	16	p-mt016	1.0000	0.0030	0.99224	0.00062	1.2500E+00
PMF-005	17	pmf005	1.0000	0.0030	1.00980	0.00065	9.8079E-01
PMF-006	18	pmf006	1.0000	0.0030	1.00235	0.00073	1.1028E+00
PMF-009	19	pmf009	1.0000	0.0027	1.00187	0.00064	1.1486E+00
PMF-010	20	pmf010	1.0000	0.0018	0.99884	0.00063	1.1977E+00
PMF-011	21	pmf011	1.0000	0.0010	0.99727	0.00079	8.4470E-02
PMF-016	22	p-mt024	1.0000	0.0038	1.00017	0.00076	8.6433E-03
	23	p-mt025	1.0000	0.0033	0.99872	0.00078	8.4271E-03
	24	p-mt026	1.0000	0.0030	0.99842	0.00079	8.0976E-03
	25	p-mt027	1.0000	0.0034	0.99750	0.00078	8.1380E-03
	26	p-mt028	1.0000	0.0032	0.99927	0.00081	8.0539E-03
PMF-017	27	p-mt029	1.0000	0.0030	0.99364	0.00066	7.7814E-01
	28	p-mt030	1.0000	0.0030	0.99832	0.00069	3.9305E-01
	29	p-mt031	1.0000	0.0030	1.00108	0.00079	2.1802E-01
	30	p-mt032	1.0000	0.0030	0.99661	0.00073	4.4129E-01
	31	p-mt033	1.0000	0.0030	1.00633	0.00076	8.8575E-02
PMF-018	32	pmf018.	1.0000	0.0030	0.99954	0.00069	9.0256E-01
PMF-019	33	pmf019.	0.9992	0.0015	1.00128	0.00065	7.6500E-01
PMF-020	34	pmf020.	0.9993	0.0015	0.99811	0.00064	1.1687E+00
PMF-021	35	pmf021_mt.	1.000	0.0026	1.00357	0.00070	7.7722E-01
PMF-022	36	pmf022_sim	1.0000	0.0021	0.99615	0.00058	1.2358E+00
PMF-023	37	pmf023_sim	1.0000	0.0020	0.99748	0.00061	1.1425E+00
PMF-024	38	pmf024_sim	1.0000	0.0021	1.00071	0.00064	6.3323E-01
PMF-025	39	pmf025_sim	1.0000	0.0020	1.00203	0.00064	1.1814E+00
PMF-026	40	pmf026_sim	1.0000	0.0020	0.99688	0.00065	1.0892E+00
PMF-027	41	pmf027_sim	1.0000	0.0020	1.00231	0.00071	7.0456E-02
PMF-028	42	pmf028_sim	1.0000	0.0024	0.99687	0.00067	1.0650E+00
PMF-029	43	pmf029_sim	1.0000	0.0022	0.99463	0.00055	1.2626E+00

Table 1: Benchmark Set 1, Pu Metal– MCNP5 Calculations

Experiment Descriptor	No.	File ID	Expt. k_{eff}	Expt. σ	MCNP k_{eff}	MCNP σ	EALF (MeV)
PMF-030	44	pmf030_sim	1.0000	0.0020	1.00124	0.00061	1.1484E+00
PMF-031	45	pmf031_sim	1.0000	0.0020	1.00189	0.00077	1.8540E-01
PMF-032	46	pmf032_sim	1.0000	0.0021	0.99689	0.00063	1.1743E+00
PMF-035	47	pmf035_shell	1.0000	0.0021	1.00766	0.00058	1.1811E+00
PMF-036	48	pmf036_shell	1.0000	0.0020	1.00383	0.00072	6.2325E-01
PMF-037	49	p-mt037	1.0000	0.0044	1.00186	0.00077	1.4627E-01
	50	p-mt038	1.0000	0.0044	0.99960	0.00076	8.5110E-02
	51	p-mt039	1.0000	0.0043	0.99944	0.00073	8.0584E-02
	52	p-mt040	1.0000	0.0043	0.99957	0.00076	7.0268E-02
	53	p-mt041	1.0000	0.0037	1.00015	0.00073	5.2879E-02
	54	p-mt042	1.0000	0.0040	0.99897	0.00079	3.1813E-02
	55	p-mt043	1.0000	0.0038	1.00048	0.00077	3.2548E-02
	56	p-mt044	1.0000	0.0033	0.99969	0.00080	1.9302E-02
	57	p-mt045	1.0000	0.0037	0.99899	0.00078	1.8910E-02
	58	p-mt046	1.0000	0.0034	1.00076	0.00074	2.5817E-02
	59	p-mt047	1.0000	0.0038	0.99497	0.00075	7.7345E-02
	60	p-mt048	1.0000	0.0040	0.99881	0.00081	2.5820E-02
	61	p-mt049	1.0000	0.0030	0.99963	0.00077	1.2321E-02
	62	p-mt050	1.0000	0.0032	1.00492	0.00078	1.5602E-02
	63	p-mt051	1.0000	0.0033	1.00117	0.00074	1.7948E-02
	64	p-mt052	1.0000	0.0039	1.00292	0.00075	2.8648E-02
PMF-039	65	pmf039_shell	1.0000	0.0022	0.98867	0.00059	1.1550E+00
PMF-040	66	pmf040_shell	1.0000	0.0038	0.99432	0.00062	1.1490E+00
PMF-041	67	pmf041_shell	1.0000	0.0016	1.00699	0.00071	1.1518E+00
		Maximum	1.00000	0.00440	1.00980	0.00081	1.27200E+00
		Minimum	0.99920	0.00100	0.98867	0.00052	8.05390E-03

Table 2: Benchmark Set 2, LEU-IEU Systems, GEMER Calculations

Experiment Descriptor (case #)	No.	File ID	Expt. k_{eff}	Expt. σ	k_{eff}	σ	H/X
Y-1948 (1)	1	Y1948-01	1	0.01000	0.99096	0.00050	420
Y-1948 (6)	2	Y1948-06	1	0.01000	0.99142	0.00057	422
Y-1948 (9)	3	Y1948-09	1	0.01000	0.98787	0.00044	500
Y-1948 (10)	4	Y1948-10	1	0.01000	0.98527	0.00043	595
LCT-033 (1)	5	LCT33-01	1	0.00380	0.99433	0.00066	196
LCT-033 (5)	6	LCT33-05	1	0.00390	0.99446	0.00067	294
LCT-033 (9)	7	LCT33-09	1	0.00400	0.99351	0.00057	407
LCT-033 (10)	8	LCT33-10	1	0.00390	0.99206	0.00058	496
LCT-033 (13)	9	LCT33-13	1	0.00410	0.99223	0.00054	613
LCT-033 (14)	10	LCT33-14	1	0.00510	0.98524	0.00045	973
LCT-033 (23)	11	LCT33-23	1	0.00400	0.99318	0.00063	196
LCT-033 (26)	12	LCT33-26	1	0.00390	0.99611	0.00068	294
LCT-033 (31)	13	LCT33-31	1	0.00390	0.99450	0.00063	407
LCT-033 (18)	14	LCT33-18	1	0.00400	0.99203	0.00068	133
LCT-033 (37)	15	LCT33-37	1	0.00410	0.99231	0.00057	496
LCT-033 (42)	16	LCT33-42	1	0.00500	0.98481	0.00048	613
LCT-033 (45)	17	LCT33-45	1	0.00380	1.00457	0.00071	973
LCT-033 (48)	18	LCT33-48	1	0.00420	1.00653	0.00067	133
ICT-001 (02)	19	ICT01-02	1	0.00400	1.00471	0.00081	16
ICT-001 (03)	20	ICT01-03	1	0.00400	0.99544	0.00097	32
ICT-001 (04)	21	ICT01-04	1	0.00400	0.99746	0.00091	64
ICT-001 (15)	22	ICT01-15	1	0.00400	0.99913	0.00095	64
ICT-001 (18)	23	ICT01-18	1	0.00400	1.00537	0.00101	32
ICT-001 (29)	24	ICT01-29	1	0.00400	1.00798	0.00089	16
LCT-045 (02)	25	LCT45-02	1	0.00244	0.99070	0.00067	71
LCT-045 (05)	26	LCT45-05	1	0.00244	0.99580	0.00075	49
LCT-045 (07)	27	LCT45-07	1	0.00213	0.99503	0.00070	77
LCT-045 (10)	28	LCT45-10	1	0.00286	0.99242	0.00076	46
LCT-045 (12)	29	LCT45-12	1	0.00239	1.00174	0.00075	98
LCT-045 (16)	30	LCT45-16	1	0.00379	1.00293	0.00070	38
LCT-045 (20)	31	LCT45-20	1	0.00291	1.00059	0.00065	78
PDK-VV-015 (10)	32	PDK15-10	1	0.01000	0.99021	0.00071	397
PDK-VV-015 (11)	33	PDK15-11	1	0.01000	0.99882	0.00064	757
PDK-VV-016 (6)	34	PDK16-06	1	0.01000	0.99743	0.00083	395
PDK-VV-016 (7)	35	PDK16-07	1	0.01000	0.99113	0.00073	504
PDK-VV-016 (7)	36	PDK16-08	1	0.01000	1.00020	0.00065	757
LCT-049 (1)	37	LCT49-01	1	0.00340	0.99607	0.00071	40
LCT-049 (9)	38	LCT49-09	1	0.00370	0.99446	0.00078	60
LCT-049 (13)	39	LCT49-13	1	0.00360	0.99750	0.00077	45
LCT-049 (16)	40	LCT49-16	1	0.00360	0.99612	0.00073	51
PDK-VV-015 (13)	41	PDK15-13	1	0.01000	0.98485	0.00079	526
PDK-VV-015 (14)	42	PDK15-14	1	0.01000	0.98725	0.00069	734
PDK-VV-015 (15)	43	PDK15-15	1	0.01000	0.98644	0.00066	999

Table 2: Benchmark Set 2, LEU-IEU Systems, GEMER Calculations

Experiment Descriptor (case #)	No.	File ID	Expt. k_{eff}	Expt. σ	k_{eff}	σ	H/X
PDK-VV-015 (16)	44	PDK15-16	1	0.01000	0.99109	0.00058	991
PDK-VV-015 (17)	45	PDK15-17	1	0.01000	0.99558	0.00066	526
PDK-VV-015 (18)	46	PDK15-18	1	0.01000	0.99411	0.00059	734
PDK-VV-015 (19)	47	PDK15-19	1	0.01000	0.99067	0.00051	1094
PDK-VV-015 (20)	48	PDK15-20	1	0.01000	0.99321	0.00050	991
PDK-VV-016 (1)	49	PDK16-01	1	0.01000	0.99958	0.00069	496
PDK-VV-016 (3)	50	PDK16-03	1	0.01000	0.98715	0.00076	646
PDK-VV-016 (4)	51	PDK16-04	1	0.01000	0.98826	0.00071	734
LCT-002 (1)	52	LST02-01	1	0.00400	0.99239	0.00049	1001
LCT-002 (2)	53	LST02-02	1	0.00370	0.99096	0.00060	1098
Y-1948 (33)	54	Y1948-33	1	0.01000	0.99634	0.00076	488
Y-1948 (37)	55	Y1948-37	1	0.01000	0.99850	0.00066	498
Y-1948 (38)	56	Y1948-38	1	0.01000	0.99903	0.00068	512
Y-1948 (39)	57	Y1948-39	1	0.01000	0.98812	0.00070	524
Y-1948 (40)	58	Y1948-40	1	0.01000	0.99938	0.00069	573
Y-1858 (A17)	59	Y1858A17	1	0.01000	0.99519	0.00075	490
LST-003 (1)	60	LST03-01	1	0.00080	0.99510	0.00060	770
LST-003 (2)	61	LST03-02	1	0.00090	0.99538	0.00063	878
LST-003 (3)	62	LST03-03	1	0.00090	0.99218	0.00062	897
LST-003 (4)	63	LST03-04	1	0.00100	0.99525	0.00056	913
LST-003 (5)	64	LST03-05	1	0.00100	0.99434	0.00055	1173
LST-003 (6)	65	LST03-06	1	0.00110	0.99493	0.00050	1213
LST-003 (7)	66	LST03-07	1	0.00110	0.99376	0.00049	1240
LST-003 (8)	67	LST03-08	1	0.00390	0.99217	0.00069	1412
LST-003 (9)	68	LST03-09	1	0.00420	0.98975	0.00060	1438
LST-004 (1)	69	LST04-01	1	0.00420	0.99486	0.00059	719
LST-004 (2)	70	LST04-02	1	0.00420	0.98805	0.00065	771
LST-004 (3)	71	LST04-03	1	0.00480	0.99128	0.00056	842
LST-004 (4)	72	LST04-04	1	0.00490	0.99058	0.00048	896
LST-004 (5)	73	LST04-05	1	0.00490	0.99025	0.00040	942
LST-004 (6)	74	LST04-06	1	0.00520	0.99397	0.00041	983
LST-004 (7)	75	LST04-07	1	0.00520	0.99158	0.00040	1018
		Maximum	1.00000	0.01000	1.00798	0.00101	1438.0
		Minimum	1.00000	0.00080	0.98481	0.00040	16.0

Table 3: USLSTATS Results Summary

Parameter	Plutonium Metal Experiments	IEU-LEU Experiments
X and range	EALF (MeV), 8.0539E-03 to 1.2720E+00	H/X, 16 – 1437.5
Administrative Margin	0.02	0.02
Average k (Unweighted)	0.99872	0.99419
Chi	4.5672 (< 9.49) - normal	5.7333 (< 9.49) - normal
Variance of fit, $s(k,X)^2$	1.4008E-05	2.1615E-05
Within variance, $s(w)^2$	9.3801E-06	4.4039E-05
Pooled variance, $s(p)^2$	2.3388E-05	6.5653E-05
Pooled std. deviation, s(p)	4.8362E-03	8.1027E-03
C(alpha,rho)*s(p)	2.0141E-02	3.4595E-02
Student-t	1.66992	1.66818
Confidence band width, W	8.2306E-03	1.4068E-02
Minimum margin of subcriticality, C*s(p)-W	1.1910E-02	2.0527E-02
Linear regression, k(X)	1.0004 + (-2.4824E-03) * X	0.9973 + (-5.6034E-06) * X
USL-1	0.9721 + (-2.4824E-03) * X (X > 0.15196) 0.9718 (X <= 0.15196)	0.9632 + (-5.6034E-06) * X
USL-2	0.9802 + (-2.4824E-03) * X (X > 1.51964E-01) 0.9799 (X <= 1.51964E-01)	0.9627 + (-5.6034E-06) * X
USL-1, range	0.9690 - 0.9718	0.9552 – 0.9631
USL-2, range	0.9771 - 0.9799	0.9546 – 0.9626

Table 4: WSMS Method Results Summary

Parameter	Plutonium Metal Experiments	IEU-LEU Experiments
X and range	EALF (MeV), 8.0539E-03 to 1.2720E+00	H/X, 16 – 1437.5
Shapiro-Wilk (Y^2/S^2, test)	0.9799 > 0.9643 - normal	0.9704 > 0.9675 - normal
Weighted average k	0.99901	0.99476
One-Sided Lower Tolerance Limit Factor	2.06500	2.06500
Average Uncertainty (σ^2)	7.0528E-06	8.4919E-06
Variance about the mean (s^2)	1.6336E-05	1.0426E-05
SQRT (Pooled Variance (S_P^2))	4.8361E-03	4.3494E-03
LTL	0.9890	0.9858
Linear regression, k(X)	1.00028 + (-1.65505E-3) * X	0.99692 + (-2.84561E-06) * X
Correlation coefficient, R^2	0.0415	0.1342
LTB	9.8817E-01 + (1.2810E-03) * X + (-1.9463E-03) * X^2	9.8619E-01 + (4.0893E-07) * X + (-2.1473E-09) * X^2
LTB range	0.9866 – 0.9883	0.9824 – 0.9862
LCB range	0.9964 – 0.9981	0.9909 – 0.9948

Table 5: GEH USLSA Results Summary

Parameter	Plutonium Metal Experiments	IEU-LEU Experiments
X and range	EALF (MeV), 8.0539E-03 to 1.2720E+00	H/X, 16 – 1437.5
Normality (Shapiro-Wilk Test), p-value	0.3557 > 0.05, normal	0.0760 > 0.05, normal
Regression model, k(X)	0.9991 + (1.3412E-05) * X	0.9962 + (-1.7503E-06) * X
Variance of fit	1.6076E-05	2.4896E-05
Within-data variance	6.9847E-06	8.4919E-06
Pooled variance	2.3061E-05	3.3388E-05
Pooled std. deviation	4.8022E-03	5.7782E-03
Correlation coefficient, R^2	0.0006	0.1411
DOF Adjusted R^2	-0.0306	0.1172
Residual Normality (Shapiro-Wilk Test), p-value	0.3569 > 0.05, normal	0.0904 > 0.05, normal
Goodness-of-fit (χ^2)	153.7489 (> 84.8206) not significant	80.5048 (< 93.9453) significant
Reduced χ_v^2	2.3654	1.1028
Model Significance F-test	0.0412 (<3.9886) not significant	11.9875 (> 3.9720) significant
SSLCB	0.9911 + (1.3412E-05) * X	0.9865 + (-1.7503E-06) * X
Confidence band width	0.0080	0.0096
Bias - Bias Uncertainty	0.0089 - (1.3412E-05) * X	-0.0135 - (-1.7503E-06) * X
Range	0.9911 – 0.9911	0.9840 – 0.9865
Extrapolated Range of X	0 – 1.3476	0 – 1484.6
SSLTB	0.9795 + (1.3412E-05) * X	0.9725 + (-1.7503E-06) * X
Tolerance band width	0.0197	0.0236
Bias - Bias Uncertainty	-0.0205 - (1.3412E-05) * X	-0.0275 - (-1.7503E-06) * X
Range	0.9795 – 0.9795	0.9700 – 0.9725
Extrapolated Range of X	0 – 1.3476	0 – 1484.6
SSLTL	0.9817	0.9732
Pooled variance, $s(p)^2$	2.2800E-05	3.4656e-05
Pooled std. deviation, s(p)	4.47749E-03	5.8870e-03
Average k	0.9987	0.9942
Tolerance band width	0.0175	0.0213
Bias - Bias Uncertainty	-0.0182	-0.0268

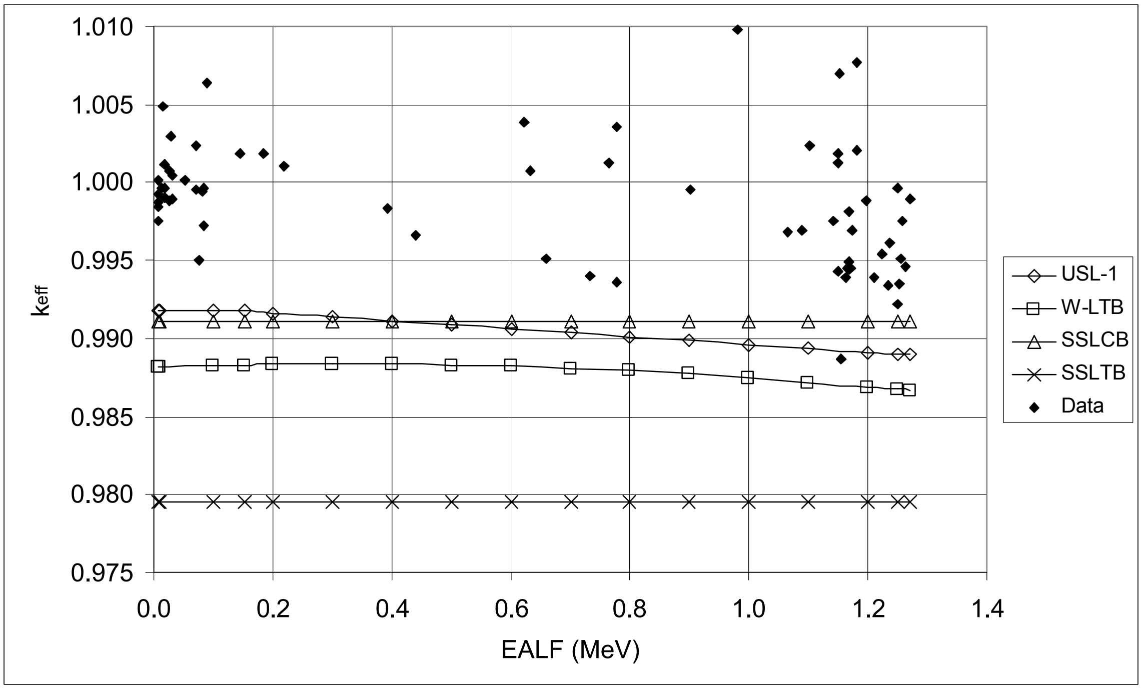

Figure 2: Comparisons of Fitted Functions for Plutonium Metal Experiments

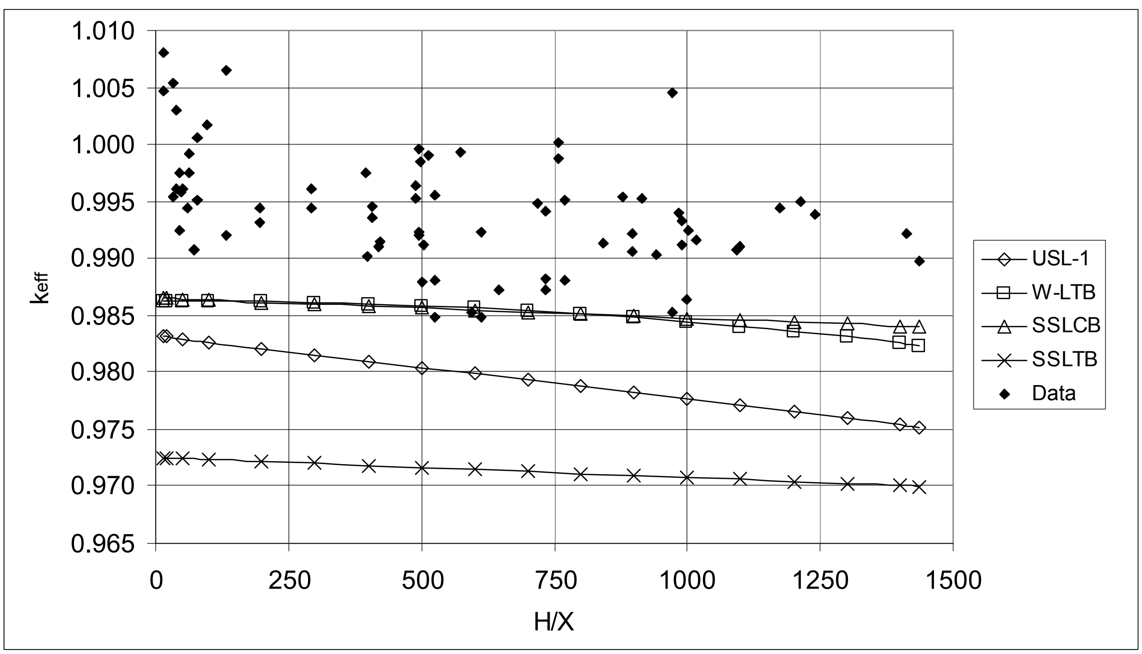

Figure 3: Comparisons of Fitted Functions for LEU-IEU Experiments